Supporting Information: Effect of truncating electrostatic interactions on predicting thermodynamic properties of water-methanol systems

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All reported excess enthalpies are reported with respect to the pure component liquids. Reported excess chemical potentials have the ideal gas phase as reference.

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Table S1. Ensemble average densities and excess enthalpies of water methanol mixture, based on the TIP4P/2005 [1] and TraPPE [2] force fields. The Ewald [3] and DSF [4] methods were used in MD simulations, using LAMMPS [5]. The densities are in units of kg.m^{-3}, and the excess enthalpies are in units of J.mol^{-1}. σ is the uncertainty.

	Ewald				DSF			
x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$
0	998.48	0.08	0	0	997.89	0.22	0	0
0.1	965.12	0.39	-269	10	964.94	0.30	-284	8
0.3	922.96	0.59	-682	13	921.90	0.23	-680	7
0.5	878.63	0.38	-671	12	877.73	0.47	-683	13
0.7	838.98	0.17	-681	7	837.64	0.19	-682	9
0.9	800.17	0.16	-323	9	798.98	0.26	-324	19
1	781.61	0.22	0	0	780.38	0.21	0	0

Table S2. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP3P [6] and TraPPE [2] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	985.3	0.4	0	0	-26017	39	–	–	1	–
0.1	950.8	0.4	-37	10	-25638	101	-20687	159	1.04	2.26
0.2	922.5	0.6	-52	13	-25251	100	-20800	302	1.10	1.95
0.3	897.4	0.2	-56	13	-24900	127	-21184	141	1.16	1.53
0.4	875.6	0.4	-52	11	-24494	101	-21228	80	1.25	1.37
0.5	855.8	0.2	-152	12	-24112	185	-21302	101	1.35	1.23
0.6	839.2	0.4	-114	14	-23726	128	-21286	126	1.46	1.15
0.7	823.1	0.5	-214	20	-23268	82	-21339	143	1.64	1.05
0.8	807.7	0.5	-154	20	-22805	171	-21240	112	1.85	1.02
0.9	793.9	0.4	-104	27	-22489	132	-21100	129	1.97	1.01
1	779.8	0.4	0	0	–	–	-20975	118	–	1

Table S3. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the SPC/E [7] and TraPPE [2] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	997.8	0.2	0	0	-30136	93	–	–	1	–
0.1	969.9	0.3	-219	18	-29848	130	-20787	285	1.01	2.18
0.2	942.8	0.4	-279	15	-29424	103	-21059	271	1.09	1.77
0.3	919.1	0.3	-327	11	-29084	152	-20977	162	1.14	1.67
0.4	895.3	0.3	-329	11	-28482	105	-21253	162	1.33	1.37
0.5	873.4	0.5	-431	22	-28097	133	-21307	73	1.43	1.23
0.6	852.2	0.6	-347	13	-27933	185	-21433	124	1.42	1.08
0.7	833.3	1.0	-449	22	-27085	154	-21423	100	1.85	1.01
0.8	814.5	0.4	-325	16	-26494	178	-21260	147	2.18	1.00
0.9	796.3	0.6	-207	22	-26359	340	-21100	102	2.16	1.00
1	779.8	0.4	0	0	–	–	-20933	133	–	1

Table S4. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the OPC [8] and TraPPE [2] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	996.9	0.8	0	0	-34278	185	–	–	1	–
0.1	966.0	0.7	-367	21	-33880	95	-20581	284	1.06	2.39
0.2	942.1	0.6	-531	16	-33545	257	-20965	243	1.10	1.86
0.3	919.3	0.3	-578	34	-33195	138	-21505	331	1.16	1.36
0.4	894.4	0.4	-588	19	-32646	206	-21439	186	1.32	1.29
0.5	875.4	0.5	-654	16	-32454	166	-21340	137	1.32	1.24
0.6	855.0	0.7	-595	28	-31687	180	-21329	204	1.66	1.15
0.7	836.6	0.3	-635	18	-31029	193	-21318	204	2.01	1.07
0.8	817.0	0.5	-421	19	-30884	359	-21392	37	1.99	0.97
0.9	798.5	0.4	-277	24	-30789	572	-21052	111	1.92	1.03
1	779.8	0.4	0	0	–	–	-20966	109	–	1

Table S5. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP4P/2005 [1] and TraPPE [2] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	996.6	0.3	0	0	-30660	165	–	–	1	–
0.1	968.6	0.5	-396	17	-30469	164	-21213	261	0.97	1.81
0.2	944.4	0.8	-564	14	-30099	113	-21332	325	1.03	1.57
0.3	921.3	0.6	-658	27	-29766	145	-21221	260	1.08	1.50
0.4	899.2	0.4	-704	22	-29432	178	-21438	210	1.13	1.26
0.5	876.3	0.4	-784	11	-28858	257	-21689	298	1.31	1.05
0.6	857.5	0.5	-705	16	-28478	154	-21573	213	1.42	1.02
0.7	837.9	0.3	-763	15	-28293	300	-21472	66	1.41	0.98
0.8	817.6	0.2	-536	25	-28058	209	-21370	118	1.45	0.95
0.9	798.7	0.7	-332	20	-27839	497	-21168	79	1.47	0.96
1	779.8	0.4	0	0	–	–	-20911	119	–	1

Table S6. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP4P/EW [9] and TraPPE [2] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

X_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle h^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	995.2	0.3	0	0	-29922	169	–	–	1	–
0.1	966.9	0.2	-311	14	-29708	183	-20724	287	0.98	2.22
0.2	942.7	0.7	-412	27	-29181	236	-21274	137	1.10	1.62
0.3	919.0	0.5	-439	13	-28764	91	-21193	317	1.19	1.53
0.4	893.7	0.5	-470	24	-28442	101	-21325	278	1.25	1.33
0.5	875.1	0.7	-584	26	-28023	236	-21704	198	1.36	1.05
0.6	853.1	0.7	-493	21	-27514	269	-21616	128	1.54	1.01
0.7	834.5	0.5	-581	20	-27158	254	-21555	132	1.65	0.96
0.8	816.2	0.5	-426	19	-26594	472	-21336	64	1.93	0.97
0.9	797.1	0.6	-258	23	-26385	234	-21019	99	1.96	1.03
1	779.8	0.4	0	0	–	–	-20932	81	–	1

Table S7. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP3P [6] and OPLS/2016 [10] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	985.3	0.4	0	0	-26000	44	–	–	1	–
0.1	946.8	0.5	268	10	-25587	29	-20807	125	1.05	2.96
0.2	913.3	0.2	457	9	-25086	84	-21500	192	1.16	2.01
0.3	884.6	0.3	596	9	-24670	84	-21956	163	1.25	1.52
0.4	860.7	0.6	674	13	-24161	61	-22171	79	1.40	1.27
0.5	841.0	0.4	609	21	-23755	58	-22266	77	1.52	1.13
0.6	824.9	0.6	606	16	-23477	93	-22308	97	1.58	1.03
0.7	812.1	0.5	440	22	-23048	66	-22141	92	1.76	1.03
0.8	801.1	0.3	381	21	-22775	106	-22036	34	1.84	1.01
0.9	791.1	0.5	210	29	-22718	271	-21992	111	1.78	0.97
1	783.3	0.6	0	0	–	–	-21781	101	–	1

Table S8. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the SPC/E [7] and OPLS/2016 [10] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	997.8	0.2	0	0	-30277	34	–	–	1	–
0.1	967.2	0.8	190	11	-29716	123	-20230	208	1.13	4.03
0.2	933.0	0.4	385	15	-29236	102	-21054	145	1.23	2.61
0.3	904.7	0.2	610	11	-28880	306	-21578	196	1.29	1.91
0.4	877.6	0.6	649	22	-28165	137	-22039	170	1.58	1.45
0.5	856.0	0.5	591	17	-27638	171	-22080	121	1.79	1.31
0.6	836.3	0.4	624	22	-27306	152	-22242	124	1.90	1.14
0.7	820.3	0.3	446	23	-26652	93	-22116	172	2.29	1.11
0.8	805.4	0.3	392	28	-26229	140	-22141	137	2.55	1.03
0.9	793.1	0.3	231	23	-25753	166	-21925	73	2.91	1.06
1	783.3	0.6	0	0	–	–	-21923	62	–	1

Table S9. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the OPC [8] and OPLS/2016 [10] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	997.8	0.2	0	0	-30277	34	–	–	1	–
0.1	967.2	0.8	190	11	-29716	123	-20230	208	1.13	4.03
0.2	933.0	0.4	385	15	-29236	102	-21054	145	1.23	2.61
0.3	904.7	0.2	610	11	-28880	306	-21578	196	1.29	1.91
0.4	877.6	0.6	649	22	-28165	137	-22039	170	1.58	1.45
0.5	856.0	0.5	591	17	-27638	171	-22080	121	1.79	1.31
0.6	836.3	0.4	624	22	-27306	152	-22242	124	1.90	1.14
0.7	820.3	0.3	446	23	-26652	93	-22116	172	2.29	1.11
0.8	805.4	0.3	392	28	-26229	140	-22141	137	2.55	1.03
0.9	793.1	0.3	231	23	-25753	166	-21925	73	2.91	1.06
1	783.3	0.6	0	0	–	–	-21923	62	–	1

Table S10. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP4P/2005 [1] and OPLS/2016 [10] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	996.6	0.3	0	0	-30714	131	–	–	1	–
0.1	969.2	0.7	-3	28	-30393	178	-19684	314	1.03	4.90
0.2	941.5	0.8	163	19	-30068	116	-20630	160	1.06	3.02
0.3	911.6	0.3	303	23	-29397	187	-21330	297	1.27	2.07
0.4	886.4	0.2	401	17	-28823	202	-21611	215	1.46	1.69
0.5	864.2	0.9	334	20	-28235	256	-21984	200	1.70	1.34
0.6	842.7	0.3	385	21	-27666	227	-21986	143	1.98	1.24
0.7	825.4	0.2	235	27	-26885	134	-22198	165	2.52	1.05
0.8	810.0	0.4	211	30	-26529	136	-21918	90	2.72	1.10
0.9	795.4	0.6	104	30	-25837	191	-22042	140	3.37	0.98
1	783.3	0.6	0	0	–	–	-21851	78	–	1

Table S11. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP4P/EW [9] and OPLS/2016 [10] force fields. The DSF [4] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

X_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	995.2	0.3	0	0	-29875	48	–	–	1	–
0.1	965.7	0.4	108	15	-29443	148	-19593	120	1.07	5.16
0.2	936.3	0.4	309	14	-29068	121	-20444	330	1.13	3.31
0.3	905.8	0.8	475	17	-28393	127	-21467	92	1.35	1.98
0.4	880.9	0.6	578	14	-27884	55	-21765	211	1.51	1.61
0.5	858.9	0.6	514	27	-27284	241	-22048	100	1.77	1.32
0.6	839.0	0.3	539	20	-26699	183	-22165	149	2.07	1.17
0.7	821.9	0.4	370	18	-25800	323	-22125	71	2.77	1.10
0.8	807.5	0.5	310	31	-25579	258	-21969	43	2.83	1.10
0.9	794.6	0.6	166	38	-24788	314	-21895	165	3.66	1.06
1	783.3	0.6	0	0	–	–	-21892	100	–	1

Table S12. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP3P [6] and TraPPE [2] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	988.1	0.2	0	8	-26077	58	–	–	1	–
0.1	953.3	0.2	-38	13	-25762	61	-20724	103	1.02	2.32
0.2	924.5	0.7	-43	20	-25426	69	-21052	149	1.05	1.84
0.3	899.1	0.3	-39	18	-25106	82	-21220	253	1.09	1.57
0.4	877.2	0.4	-28	21	-24574	75	-21340	121	1.24	1.37
0.5	857.4	0.2	-106	23	-24047	121	-21248	177	1.42	1.31
0.6	839.7	0.2	-73	28	-23677	122	-21451	93	1.53	1.12
0.7	823.8	0.4	-180	27	-23318	242	-21262	95	1.64	1.12
0.8	808.6	0.3	-102	28	-22869	35	-21289	146	1.84	1.04
0.9	794.5	0.2	-74	30	-22713	166	-21098	55	1.84	1.05
1	781.4	0.5	0	43	–	–	-21075	123	–	1

Table S13. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the SPC/E [7] and TraPPE [2] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	1000.1	0.6	0	28	-30159	248	–	–	1	–
0.1	972.1	0.3	-221	23	-29982	128	-20443	291	0.97	2.54
0.2	945.7	0.4	-281	22	-29581	153	-20613	269	1.03	2.15
0.3	920.5	0.2	-321	24	-29143	225	-21322	148	1.12	1.47
0.4	896.3	0.3	-303	23	-28854	134	-21358	124	1.16	1.33
0.5	875.2	0.6	-408	36	-28098	164	-21367	123	1.45	1.21
0.6	854.3	1.0	-358	34	-27943	268	-21315	98	1.42	1.15
0.7	833.4	0.4	-390	29	-27536	309	-21325	96	1.55	1.06
0.8	815.8	0.7	-296	29	-26706	282	-21250	128	2.02	1.02
0.9	797.5	0.7	-171	33	-26518	512	-21212	152	2.04	0.97
1	781.4	0.5	0	43	–	–	-20965	92	–	1

Table S14. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the OPC [8] and TraPPE [2] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	1004.1	1.0	0	0	-34581	149	–	–	1	–
0.1	971.2	0.8	-312	24	-34101	176	-20033	529	1.09	3.14
0.2	944.7	0.4	-443	24	-33632	168	-20411	288	1.20	2.45
0.3	921.4	0.7	-460	29	-33292	230	-21111	150	1.26	1.68
0.4	897.9	0.4	-479	27	-32944	337	-21223	278	1.32	1.48
0.5	876.9	0.4	-563	27	-32517	333	-21569	139	1.44	1.18
0.6	855.9	0.9	-436	41	-31682	580	-21356	173	1.88	1.19
0.7	837.9	0.8	-526	36	-31435	208	-21617	182	1.92	0.99
0.8	818.4	0.3	-342	35	-31144	227	-21351	138	2.01	1.03
0.9	799.1	0.4	-190	33	-30339	297	-21232	94	2.60	1.01
1	781.4	0.5	0	0	–	–	-21085	57	–	1

Table S15. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP4P/2005 [1] and TraPPE [2] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	1001.6	0.6	0	0	-30974	121	–	–	1	–
0.1	972.1	0.2	-355	20	-30615	247	-20799	804	1.04	2.22
0.2	947.7	0.7	-519	29	-30318	307	-21370	182	1.07	1.60
0.3	923.7	0.7	-591	30	-30119	245	-21387	182	1.06	1.45
0.4	901.7	0.2	-655	29	-29529	282	-21566	349	1.23	1.24
0.5	879.1	0.4	-700	24	-29142	234	-21626	219	1.32	1.11
0.6	859.4	0.5	-655	30	-28818	112	-21709	118	1.39	1.00
0.7	839.2	0.6	-715	32	-28379	176	-21575	151	1.54	0.97
0.8	819.3	0.9	-523	33	-28108	109	-21269	81	1.60	1.03
0.9	799.5	0.5	-299	31	-27515	410	-21229	120	1.89	0.97
1	781.4	0.5	0	0	–	–	-20988	76	–	1

Table S16. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP4P/EW [9] and TraPPE [2] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

X_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle h^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	999.0	0.9	0	0	-30103	172	–	–	1	–
0.1	971.1	0.4	-267	22	-29799	112	-20630	234	1.02	2.39
0.2	945.5	0.5	-383	29	-29415	182	-21028	208	1.08	1.85
0.3	921.1	0.3	-401	22	-28889	217	-21121	314	1.22	1.63
0.4	897.2	0.6	-427	28	-28636	218	-21579	221	1.24	1.24
0.5	874.8	1.0	-494	35	-28048	267	-21535	109	1.44	1.16
0.6	855.6	0.4	-436	29	-27892	323	-21777	241	1.42	0.98
0.7	836.0	0.9	-521	34	-27016	302	-21449	220	1.88	1.03
0.8	816.4	0.5	-372	32	-26918	331	-21387	153	1.82	0.98
0.9	798.9	0.4	-230	33	-26485	555	-21264	175	2.02	0.96
1	781.4	0.5	0	0	–	–	-21009	85	–	1

Table S17. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP3P [6] and OPLS/2016 [10] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	988.1	0.2	0	0	-26072	62	–	–	1	–
0.1	948.9	0.3	259	11	-25719	71	-20739	183	1.03	3.07
0.2	914.8	0.5	486	11	-25331	87	-21519	181	1.08	2.02
0.3	886.0	0.2	613	13	-24752	78	-21930	143	1.24	1.55
0.4	862.0	0.5	686	18	-24446	164	-22160	75	1.28	1.29
0.5	842.7	0.5	621	19	-23943	98	-22335	173	1.45	1.11
0.6	826.1	0.3	646	15	-23470	142	-22343	153	1.63	1.03
0.7	812.6	0.3	470	16	-23050	125	-22171	97	1.80	1.03
0.8	801.7	0.5	395	17	-22780	340	-22083	180	1.89	1.00
0.9	792.2	0.4	223	19	-22534	258	-22000	113	1.96	0.98
1	783.8	0.5	0	0	–	–	-21806	49	–	1

Table S18. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the SPC/E [7] and OPLS/2016 [10] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	1000.1	0.6	0	0	-30354	49	–	–	1	–
0.1	969.4	0.3	186	21	-29929	76	-20256	149	1.07	3.89
0.2	936.7	0.2	435	19	-29455	356	-21042	241	1.17	2.55
0.3	905.9	0.4	601	18	-28969	141	-21686	152	1.28	1.78
0.4	878.9	0.6	683	17	-28250	143	-22052	166	1.57	1.41
0.5	856.8	0.4	625	20	-27703	144	-22097	45	1.80	1.27
0.6	837.9	0.2	654	20	-27192	250	-22076	79	2.04	1.18
0.7	821.1	0.5	470	18	-26443	234	-22214	121	2.57	1.04
0.8	806.8	0.4	396	18	-26352	251	-21993	48	2.50	1.07
0.9	794.4	0.2	213	21	-25830	240	-22002	88	2.90	1.00
1	783.8	0.5	0	0	–	–	-21856	138	–	1

Table S19. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the OPC [8] and OPLS/2016 [10] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	1004.1	1.0	0	0	-34491	182	–	–	1	–
0.1	973.1	0.2	-87	13	-34110	182	-19852	172	1.05	4.70
0.2	944.1	0.3	-20	22	-33473	254	-20813	386	1.23	2.89
0.3	916.7	0.2	87	16	-33228	75	-21234	136	1.23	2.22
0.4	891.6	1.0	138	24	-32428	290	-21749	96	1.56	1.65
0.5	868.6	0.4	91	16	-32280	543	-22095	233	1.52	1.31
0.6	848.2	0.3	121	18	-31393	240	-22238	150	2.01	1.15
0.7	829.0	0.9	-4	35	-30371	316	-22215	116	2.81	1.08
0.8	812.2	0.3	43	16	-30253	220	-22022	138	2.76	1.09
0.9	797.3	0.2	20	18	-29908	177	-21965	57	2.97	1.04
1	783.8	0.5	0	0	–	–	-21914	143	–	1

Table S20. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP4P/2005 [1] and OPLS/2016 [10] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

x_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle\bar{h}^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	1001.6	0.6	0	0	-30964	187	–	–	1	–
0.1	973.2	0.7	32	17	-30612	104	-19509	604	1.04	5.26
0.2	941.9	0.3	213	27	-30150	117	-20620	190	1.13	3.03
0.3	914.0	0.5	376	18	-29653	192	-21390	84	1.26	2.02
0.4	888.8	0.6	452	22	-29071	211	-21733	162	1.46	1.61
0.5	865.2	0.3	410	23	-28501	288	-22068	161	1.68	1.29
0.6	845.6	0.5	437	19	-27670	274	-22096	93	2.18	1.18
0.7	827.4	0.2	267	22	-27227	134	-22135	54	2.42	1.08
0.8	810.7	0.3	263	21	-26610	197	-22145	100	2.90	1.00
0.9	796.3	0.4	125	16	-25943	196	-22044	104	3.55	0.98
1	783.8	0.5	0	0	–	–	-21844	127	–	1

Table S21. Ensemble average densities, excess enthalpies, excess chemical potentials and activity coefficients of water and methanol, based on the TIP4P/EW [9] and OPLS/2016 [10] force fields. The Wolf [11] method was used to calculate the electrostatic interactions. The densities are in units of kg.m^{-3}. The excess mixing enthalpies and the excess chemical potentials are in units of J.mol^{-1}. σ is the uncertainty.

X_{MeOH}	$\langle\rho\rangle_{\mathrm{NPT}}$	σ_ρ	$\langle h^{\mathrm{ex}}\rangle_{\mathrm{NPT}}$	$\sigma_{h^{\mathrm{ex}}}$	$\mu^{\mathrm{ex}}_{\mathrm{H_2O}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{H_2O}}}$	$\mu^{\mathrm{ex}}_{\mathrm{MeOH}}$	$\sigma_{\mu^{\mathrm{ex}}_{\mathrm{MeOH}}}$	$\gamma_{\mathrm{H_2O}}$	γ_{MeOH}
0	999.0	0.9	0	0	-29976	256	–	–	1	–
0.1	970.1	0.5	148	16	-29699	192	-19358	328	1.01	5.88
0.2	938.2	0.5	365	17	-29234	200	-20654	109	1.10	3.15
0.3	910.0	0.5	538	22	-28733	155	-21141	246	1.22	2.35
0.4	883.3	0.6	624	17	-28043	121	-21760	222	1.47	1.67
0.5	860.6	0.3	586	16	-27263	181	-22094	179	1.85	1.34
0.6	841.6	0.1	581	17	-26871	250	-21940	117	2.01	1.32
0.7	823.7	0.2	398	17	-26180	319	-22205	109	2.47	1.10
0.8	808.5	0.4	354	25	-25569	267	-22067	274	2.95	1.09
0.9	795.0	0.3	187	20	-25272	176	-22180	162	3.12	0.98
1	783.8	0.5	0	0	–	–	-21979	125	–	1

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